# ON SIMULATIONS OF THE CLASSICAL HARMONIC OSCILLATOR EQUATION BY DIFFERENCE EQUATIONS

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We discuss the discretizations of the second-order linear ordinary diffrential equations with constant coefficients. Special attention is given to the exact discretization because there exists a difference equation whose solutions exactly coincide with solutions of the corresponding differential equation evaluated at a discrete sequence of points. Such exact discretization can be found for an arbitrary lattice spacing.

## 1. Introduction

The motivation for writing this paper is an observation that small and apparently not very important changes in the discretization of a differential equation lead to difference equations with completely different properties. By the discretization we mean a simulation of the differential equation by a difference equation [5].

In this paper we consider the damped harmonic oscillator equation

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2 x = 0, \tag{1.1}$$

where $x = x(t)$ and the dot means the $t$-derivative. This is a linear equation and its general solution is well known. Therefore discretization procedures are not so important (but sometimes are applied, see [3]). However, this example allows us to show and illustrate some more general ideas.

The most natural discretization, known as the Euler method (Appendix B, cf. [5, 10]) consists in replacing $x$ by $x_n$, $\dot{x}$ by the difference ratio $(x_{n+1} - x_n)/\varepsilon$, $\ddot{x}$ by the difference ratio of difference ratios, that is,

$$\ddot{x} \longrightarrow \frac{1}{\varepsilon}\left(\frac{x_{n+2} - x_{n+1}}{\varepsilon} - \frac{x_{n+1} - x_n}{\varepsilon}\right) = \frac{x_{n+2} - 2x_{n+1} + x_n}{\varepsilon^2}, \tag{1.2}$$

and so on. This possibility is not unique. We can replace, for instance, $x$ by $x_{n+1}$, $\dot{x}$ by $(x_n - x_{n-1})/\varepsilon$, or $\ddot{x}$ by $(x_{n+1} - 2x_n + x_{n-1})/\varepsilon^2$. Actually the last formula, due to its symmetry, seems to be more natural than (1.2) (and it works better indeed, see Section 2).

In any case we demand that the continuum limit, that is,

$$x_n = x(t_n), \quad t_n = \varepsilon n, \; \varepsilon \longrightarrow 0, \tag{1.3}$$

applied to any discretization of a differential equation yields this differential equation. The continuum limit consists in replacing $x_n$ by $x(t_n) = x(t)$ and the neighboring values are computed from the Taylor expansion of the function $x(t)$ at $t = t_n$:

$$x_{n+k} = x(t_n + k\varepsilon) = x(t_n) + \dot{x}(t_n)k\varepsilon + \frac{1}{2}\ddot{x}(t_n)k^2\varepsilon^2 + \cdots. \tag{1.4}$$

Substituting these expansions into the difference equation and leaving only the leading term we should obtain the considered differential equation.

In this paper we compare various discretizations of the damped (and undamped) harmonic oscillator equation, including the exact discretization of the damped harmonic oscillator equation (1.1). By exact discretization we mean that $x_n = x(t_n)$ holds for any $\varepsilon$ and not only in the limit (1.3).

## 2. Simplest discretizations of the harmonic oscillator

Let us consider the following three discrete equations:

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\varepsilon^2} + x_{n-1} = 0, \tag{2.1}$$

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\varepsilon^2} + x_n = 0, \tag{2.2}$$

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\varepsilon^2} + x_{n+1} = 0, \tag{2.3}$$

where $\varepsilon$ is a constant. The continuum limit (1.3) yields, in any of these cases, the harmonic oscillator equation

$$\ddot{x} + x = 0. \tag{2.4}$$

To fix our attention, in this paper we consider only the solutions corresponding to the initial conditions $x(0) = 0$, $\dot{x}(0) = 1$. The initial data for the discretizations are chosen in the simplest form: we assume that $x_0$ and $x_1$ belong to the graph of the exact continuous solution.

For small $t_n$ and small $\varepsilon$, the discrete solutions of any of these equations approximate the corresponding continuous solution quite well (see Figure 2.1). However, the global behaviors of the solutions (still for small $\varepsilon$!) are different (see Figure 2.2). The solution of (2.3) vanishes at $t \to \infty$, while the solution of (2.1) oscillates with rapidly increasing amplitude (all black points are outside the range of Figure 2.2). Qualitatively, only the discretization (2.2) resembles the continuous case. However, for very large $t$ the discrete
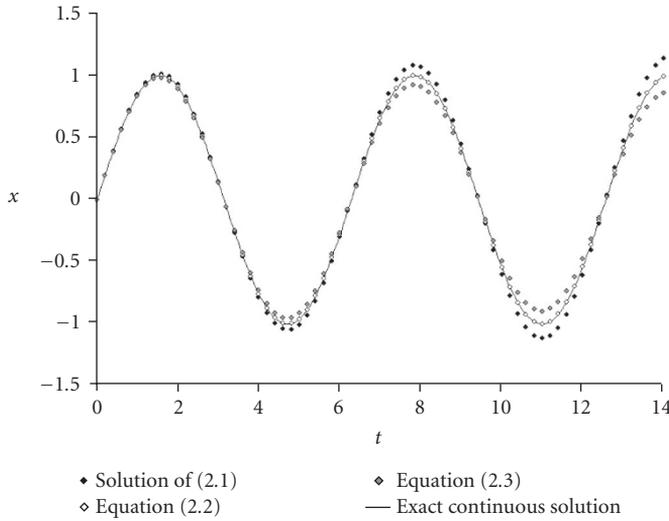
Figure 2.1.  Simplest discretizations of the harmonic oscillator equation for small $t$ and $\varepsilon = 0.02$.

solution becomes increasingly different from the exact continuous solution even in the case (2.2) (cf. Figures 2.2 and 2.3).

The natural question arises: *how to find a discretization which is the best as far as global properties of solutions are concerned?*

In this paper we will show how to find the "exact" discretization of the damped harmonic oscillator equation. In particular, we will present the discretization of (2.4) which is better than (2.2) and, in fact, seems to be the best possible. We begin, however, with a very simple example which illustrates the general idea of this paper quite well.

## 3. The exact discretization of the exponential growth equation

We consider the discretization of the equation $\dot{x} = x$. Its general solution reads

$$x(t) = x(0)e^t. \tag{3.1}$$

The simplest discretization is given by

$$\frac{x_{n+1} - x_n}{\varepsilon} = x_n. \tag{3.2}$$

This discrete equation can be solved immediately. Actually this is just the geometric sequence $x_{n+1} = (1 + \varepsilon)x_n$. Therefore

$$x_n = (1 + \varepsilon)^n x_0. \tag{3.3}$$

To compare with the continuous case we write $(1 + \varepsilon)^n$ in the form

$$(1 + \varepsilon)^n = \exp\left(n\ln(1 + \varepsilon)\right) = \exp\left(\kappa t_n\right), \tag{3.4}$$
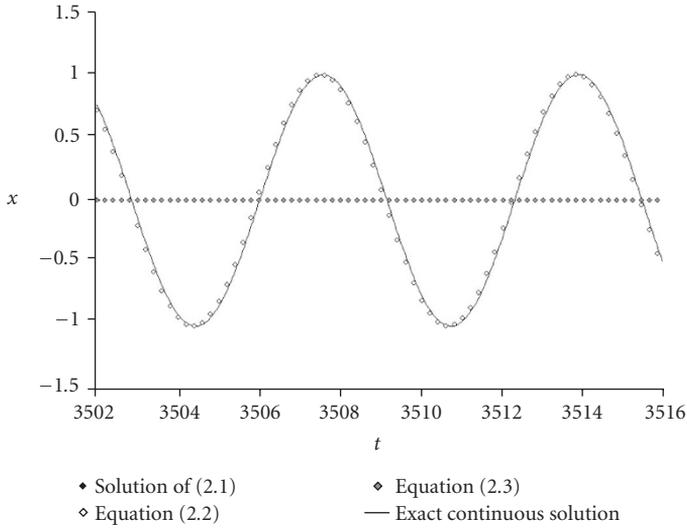
Figure 2.2.  Simplest discretizations of the harmonic oscillator equation for large $t$ and $\varepsilon = 0.02$.
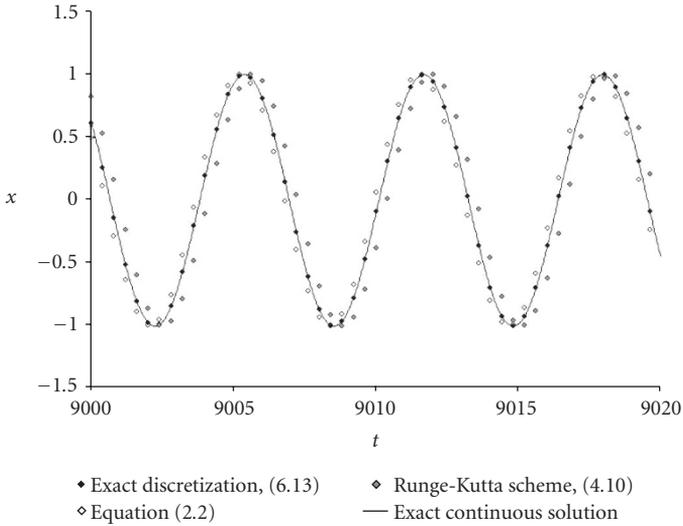


Figure 2.3.  Good discretizations of the harmonic oscillator equation for large $t$ and $\varepsilon = 0.02$.

where $t_n := \varepsilon n$ and $\kappa := \varepsilon^{-1} \ln(1 + \varepsilon)$. Thus the solution (3.3) can be rewritten as

$$x_n = x_0 e^{\kappa t_n}. \tag{3.5}$$

Therefore we see that for $\kappa \neq 1$ the continuous solution (3.1), evaluated at $t_n$, that is,

$$x(t_n) = x(0)e^{t_n}, \tag{3.6}$$

differs from the corresponding discrete solution (3.5). One can easily see that $0 < \kappa < 1$. Only in the limit $\varepsilon \to 0$ we have $\kappa \to 1$.

Although the qualitative behavior of the "naive" simulation (3.2) is in good agreement with the smooth solution (exponential growth in both cases), but quantitatively the discrepancy is very large for $t \to \infty$ because the exponents are different.

The discretization (3.2) can be easily improved. Indeed, replacing in the formula (3.3) $1 + \varepsilon$ by $e^\varepsilon$ we obtain that it coincides with the exact solution (3.6). This "exact discretization" is given by

$$\frac{x_{n+1} - x_n}{e^\varepsilon - 1} = x_n, \tag{3.7}$$

or, simply, $x_{n+1} = e^\varepsilon x_n$. Note that $e^\varepsilon \approx 1 + \varepsilon$ (for $\varepsilon \approx 0$) and this approximation yields (3.2).

## 4. Discretizations of the harmonic oscillator: exact solutions

The general solution of the harmonic oscillator equation (2.4) is well known:

$$x(t) = x(0)\cos t + \dot{x}(0)\sin t. \tag{4.1}$$

In Section 2 we compared graphically this solution with the simplest discrete simulations: (2.1), (2.2), (2.3). Now we are going to present exact solutions of these discrete equations.

Because the discrete case is usually less known than the continuous one, we recall shortly that the simplest approach consists in searching solutions in the form $x_n = \Lambda^n$ (this is an analogue of the ansatz $x(t) = \exp(\lambda t)$ made in the continuous case, for more details, see Appendix A). As a result we get the characteristic equation for $\Lambda$.

We illustrate this approach on the example of (2.1) resulting from the Euler method. Substituting $x_n = \Lambda^n$ we get the following characteristic equation:

$$\Lambda^2 - 2\Lambda + (1 + \varepsilon^2) = 0, \tag{4.2}$$

with solutions $\Lambda_1 = 1 + i\varepsilon$, $\Lambda_2 = 1 - i\varepsilon$. The general solution of (2.1) reads

$$x_n = c_1 \Lambda_1^n + c_2 \Lambda_2^n, \tag{4.3}$$

and, expressing $c_1$, $c_2$ by the initial conditions $x_0$, $x_1$, we have

$$x_n = x_1 \frac{(1 + i\varepsilon)^n - (1 - i\varepsilon)^n}{2i\varepsilon} + x_0 \frac{(1 + i\varepsilon)(1 - i\varepsilon)^n - (1 - i\varepsilon)(1 + i\varepsilon)^n}{2i\varepsilon}. \tag{4.4}$$

Denoting

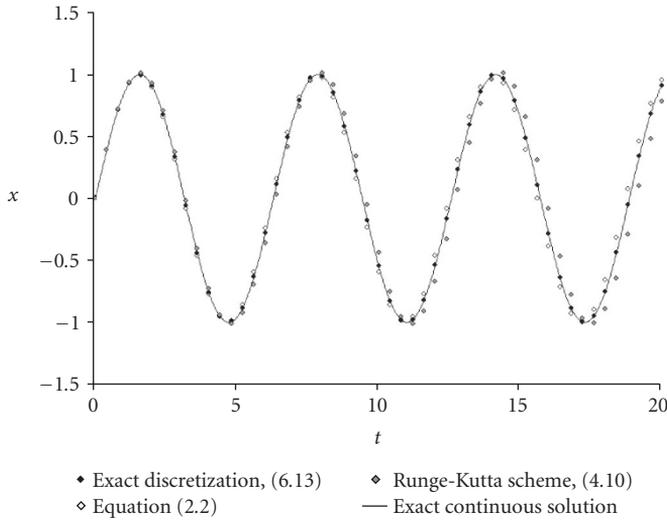$$1 + i\varepsilon = \rho e^{i\alpha}, \tag{4.5}$$

Figure 4.1. Good discretizations of the harmonic oscillator equation for small $t$ and $\varepsilon = 0.4$.

where $\rho = \sqrt{1 + \varepsilon^2}$ and $\alpha = \arctan \varepsilon$, we obtain after elementary calculations

$$x_n = \rho^n \left( x_0 \cos(n\alpha) + \frac{x_1 - x_0}{\varepsilon} \sin(n\alpha) \right). \tag{4.6}$$

It is convenient to denote $\rho = e^{\kappa \varepsilon}$ and

$$t_n = n\varepsilon, \qquad \kappa := \frac{1}{2\varepsilon} \ln \left(1 + \varepsilon^2\right), \qquad \omega := \frac{\arctan \varepsilon}{\varepsilon}, \tag{4.7}$$

and then

$$x_n = e^{\kappa t_n} \left( x_0 \cos \omega t_n + \frac{x_1 - x_0}{\varepsilon} \sin \omega t_n \right). \tag{4.8}$$

One can check that $\kappa > 0$ and $\omega < 1$ for any $\varepsilon > 0$. For $\varepsilon \to 0$ we have $\kappa \to 0$, $\omega \to 1$. Therefore the discrete solution (4.8) is characterized by the exponential growth of the envelope amplitude and a smaller frequency of oscillations than the corresponding continuous solution (4.1).

A similar situation is in the case (2.3), with only one (but very important) difference: instead of the growth we have the exponential decay. The formulas (4.7) and (4.8) need only one correction to be valid in this case. Namely, $\kappa$ has to be changed to $-\kappa$.

The third case, (2.2), is characterized by $\rho = 1$, and, therefore, the amplitude of the oscillations is constant (this case will be discussed below in more detail).

These results are in perfect agreement with the behavior of the solutions of discrete equations illustrated in Figures 2.1 and 2.2.

Let us consider the following family of discrete equations (parameterized by real parameters $p$, $q$):

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\varepsilon^2} + px_{n-1} + (1 - p - q)x_n + qx_{n+1} = 0. \tag{4.9}$$

The continuum limit (1.3) applied to (4.9) yields the harmonic oscillator (2.4) for any $p$, $q$. The family (4.9) contains all three examples of Section 2 and (for $p = q = 1/4$) the equation resulting from the Gauss-Legendre-Runge-Kutta method (see Appendix B):

$$x_{n+1} - 2\left(\frac{4 - \varepsilon^2}{4 + \varepsilon^2}\right)x_n + x_{n-1} = 0. \tag{4.10}$$

Substituting $x_n = \Lambda^n$ into (4.9) we get the following characteristic equation:

$$(1 + q\varepsilon^2)\Lambda^2 - (2 + (p + q - 1)\varepsilon^2)\Lambda + (1 + p\varepsilon^2) = 0. \tag{4.11}$$

We formulate the following problem: *find a discrete equation in the family (4.9) with the global behavior of solutions as much similar to the continuous case as possible.*

At least two conditions seem to be very natural in order to get a "good" discretization of the harmonic oscillator: oscillatory character and a constant amplitude of the solutions (i.e., $\rho = 1$, $\kappa = 0$). These conditions can be easily expressed in terms of roots ($\Lambda_1$, $\Lambda_2$) of the quadratic equation (4.11). First, the roots should be imaginary (i.e., $\Delta < 0$), second, their modulus should be equal to 1, that is, $\Lambda_1 = e^{i\alpha}$, $\Lambda_2 = e^{-i\alpha}$. Therefore $1 + p\varepsilon^2 = 1 + q\varepsilon^2$, that is, $q = p$. In the case $q = p$, the discriminant $\Delta$ of the quadratic equation (4.11) is given by

$$\Delta = -4\varepsilon^2 + \varepsilon^4(1 - 4p). \tag{4.12}$$

There are two possiblities: if $p \geq 1/4$, then $\Delta < 0$ for any $\varepsilon \neq 0$, and if $p < 1/4$, then $\Delta < 0$ for sufficiently small $\varepsilon$, namely $\varepsilon^2 < 4(1 - 4p)^{-1}$. In any case, these requirements are not very restrictive and we obtained $p$-family of good discretizations of the harmonic oscilltor. If $\Lambda_1 = e^{i\alpha}$ and $\Lambda_2 = e^{-i\alpha}$, then the solution of (4.9) is given by

$$x_n = x_0 \cos(t_n\omega) + \frac{x_1 - x_0 \cos\alpha}{\sin\alpha} \sin(t_n\omega), \tag{4.13}$$

where $\omega = \alpha/\varepsilon$, that is,

$$\omega = \frac{1}{\varepsilon} \arctan\left(\varepsilon \frac{\sqrt{1 + \varepsilon^2(p - 1/4)}}{1 + (p - 1/2)\varepsilon^2}\right). \tag{4.14}$$

Note that the formula (4.13) is invariant with respect to the transformation $\alpha \to -\alpha$ which means that we can choose $\Lambda_1$ as any of the two roots of (4.11).

Equation (2.2) is a special case of (4.9) for $q = p = 0$. As we have seen in Section 2, for small $\varepsilon$ this discretization simulates the harmonic oscillator (2.4) much better than (2.1) or (2.3). However, for sufficiently large $\varepsilon$ (namely, $\varepsilon > 2$), the properties of this discretization change dramatically. Its generic solution grows exponentially without oscillations.

Expanding (4.14) in the Maclaurin series with respect to $\varepsilon$, we get

$$\omega \approx 1 + \frac{1 - 12p}{24}\varepsilon^2 + \frac{3 - 40p + 240p^2}{640}\varepsilon^4 + \cdots. \tag{4.15}$$

Therefore the best approximation of (2.4) from among the family (4.9) is characterized by $p = 1/12$:

$$x_{n+1} - 2\left(\frac{12 - 5\varepsilon^2}{12 + \varepsilon^2}\right)x_n + x_{n-1} = 0. \tag{4.16}$$

In this case $\omega \approx 1 + \varepsilon^4/480 + \cdots$ is closest to the exact value $\omega = 1$.

The standard numerical methods give similar results (in all cases presented in Appendix B, the discretization of the second derivative is the simplest one, the same as described in our introduction). The corresponding discrete equations do not simulate (2.4) better than the discretizations presented in Section 2.

## 5. Damped harmonic oscillator and its discretization

Let us consider the damped harmonic oscillator equation (1.1). Its general solution can be expressed by the roots $\lambda_1$, $\lambda_2$ of the characteristic equation $\lambda^2 + 2\gamma\lambda + \omega_0^2 = 0$ and the initial data $x(0)$, $\dot{x}(0)$:

$$x(t) = \left(\frac{\dot{x}(0) - \lambda_2 x(0)}{\lambda_1 - \lambda_2}\right)e^{\lambda_1 t} + \left(\frac{\dot{x}(0) - \lambda_1 x(0)}{\lambda_2 - \lambda_1}\right)e^{\lambda_2 t}. \tag{5.1}$$

In the weakly damped case ($\omega_0 > \gamma > 0$), we have $\lambda_1 = -\gamma + i\omega$ and $\lambda_2 = -\gamma - i\omega$, where $\omega = \sqrt{\omega_0^2 - \gamma^2}$. Then

$$x(t) = x(0)e^{-\gamma t}\cos\omega t + \omega^{-1}(\dot{x}(0) + \gamma x(0))e^{-\gamma t}\sin\omega t. \tag{5.2}$$

To obtain some simple discretization of (1.1), we should replace the first derivative and the second derivative by discrete analogues. The results of Section 2 suggest that the best way to discretize the second derivative is the symmetric one, like in (2.2). There are at least 3 possibilities for the discretization of the first derivative leading to the following simulations of the damped harmonic oscillator equation:

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\varepsilon^2} + 2\gamma\frac{x_n - x_{n-1}}{\varepsilon} + \omega_0^2 x_n = 0, \tag{5.3}$$

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\varepsilon^2} + 2\gamma\frac{x_{n+1} - x_{n-1}}{2\varepsilon} + \omega_0^2 x_n = 0, \tag{5.4}$$

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\varepsilon^2} + 2\gamma\frac{x_{n+1} - x_n}{\varepsilon} + \omega_0^2 x_n = 0. \tag{5.5}$$

As one could expect, the best simulation is given by the most symmetric equation, that is, (5.4), see Figure 5.1.
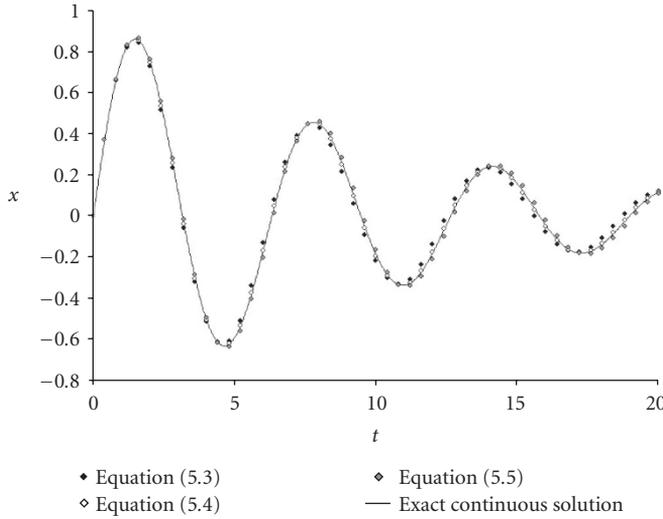
Figure 5.1.  Simplest discretizations of the weakly damped harmonic oscillator equation ($\omega_0 = 1$, $\gamma = 0.1$) for small $t$ and $\varepsilon = 0.3$.

## 6. The exact discretization of the damped harmonic oscillator equation

In order to find the exact discretization of (1.1) we consider the general linear discrete equation of second order:

$$x_{n+2} = 2Ax_{n+1} + Bx_n. \tag{6.1}$$

The general solution of (6.1) has the following closed form (cf. Appendix A):

$$x_n = \frac{x_0\left(\Lambda_1\Lambda_2^n - \Lambda_2\Lambda_1^n\right) + x_1\left(\Lambda_1^n - \Lambda_2^n\right)}{\Lambda_1 - \Lambda_2}, \tag{6.2}$$

where $\Lambda_1$, $\Lambda_2$ are roots of the characteristic equation $\Lambda^2 - 2A\Lambda - B = 0$, that is,

$$\Lambda_1 = A + \sqrt{A^2 + B}, \qquad \Lambda_2 = A - \sqrt{A^2 + B}. \tag{6.3}$$

The formula (6.2) is valid for $\Lambda_1 \neq \Lambda_2$, which is equivalent to $A^2 + B \neq 0$. If the eigenvalues coincide ($\Lambda_2 = \Lambda_1$, $B = -A^2$), we have $\Lambda_1 = A$ and

$$x_n = (1 - n)\Lambda_1^n x_0 + n\Lambda_1^{n-1}x_1. \tag{6.4}$$

*Is it possible to identify $x_n$ given by (6.2) with $x(t_n)$ where $x(t)$ is given by (5.1)?*
    Yes! It is sufficient to express in an appropriate way $\lambda_1$ and $\lambda_2$ by $\Lambda_1$ and $\Lambda_2$ and also the initial conditions $x(0)$, $\dot{x}(0)$ by $x_0$, $x_1$. It is quite surprising that the above identification can be done for any $\varepsilon$.

The crucial point consists in setting

$$\Lambda_k^n = \exp\left(n\ln\Lambda_k\right) = \exp\left(t_n\lambda_k\right),\qquad(6.5)$$

where, as usual, $t_n := n\varepsilon$. It means that

$$\lambda_k := \varepsilon^{-1}\ln\Lambda_k\qquad(6.6)$$

(note that for imaginary $\Lambda_k$, say $\Lambda_k = \rho_k e^{i\alpha_k}$, we have $\ln\Lambda_k = \ln\rho_k + i\alpha_k$). Then (6.2) assumes the form

$$x_n = \left(\frac{x_1 - x_0 e^{\varepsilon\lambda_2}}{e^{\varepsilon\lambda_1} - e^{\varepsilon\lambda_2}}\right)e^{\lambda_1 t_n} + \left(\frac{x_1 - x_0 e^{\varepsilon\lambda_1}}{e^{\varepsilon\lambda_2} - e^{\varepsilon\lambda_1}}\right)e^{\lambda_2 t_n}.\qquad(6.7)$$

Comparing (5.1) with (6.7) we get $x_n = x(t_n)$ provided that

$$x(0) = x_0,\qquad \dot{x}(0) = \frac{(\lambda_1 - \lambda_2)x_1 - (\lambda_1 e^{\varepsilon\lambda_2} - \lambda_2 e^{\varepsilon\lambda_1})x_0}{e^{\varepsilon\lambda_1} - e^{\varepsilon\lambda_2}}.\qquad(6.8)$$

The degenerate case, $\Lambda_1 = \Lambda_2$ (which is equivalent to $\lambda_1 = \lambda_2$) can be considered analogically (cf. Appendix A). The formula (6.4) is obtained from (6.2) in the limit $\Lambda_2 \to \Lambda_1$. Therefore all formulas for the degenerate case can be derived simply by taking the limit $\lambda_2 \to \lambda_1$.

Thus we have a one-to-one correspondence between second-order differential equations with constant coefficients and second-order discrete equations with constant coefficients. This correspondence, referred to as the exact discretization, is induced by the relation (6.6) between the eigenvalues of the associated characteristic equations.

The damped harmonic oscillator (1.1) corresponds to the discrete equation (6.1) such that

$$2A = e^{-\varepsilon\gamma}\left(e^{\varepsilon\sqrt{\gamma^2 - \omega_0^2}} + e^{-\varepsilon\sqrt{\gamma^2 - \omega_0^2}}\right),\qquad B = -e^{-2\varepsilon\gamma}.\qquad(6.9)$$

In the case of the weakly damped harmonic oscillator ($\omega_0 > \gamma > 0$), the exact discretization is given by

$$A = e^{-\varepsilon\gamma}\cos(\varepsilon\omega),\qquad B = -e^{-2\varepsilon\gamma},\qquad(6.10)$$

where $\omega := \sqrt{\omega_0^2 - \gamma^2}$. In other words, the exact discretization of (1.1) reads

$$x_{n+2} - 2e^{-\varepsilon\gamma}\cos(\omega\varepsilon)x_{n+1} + e^{-2\gamma\varepsilon}x_n = 0.\qquad(6.11)$$

The initial data are related as follows (see (6.8)):

$$x(0) = x_0,\qquad \dot{x}(0) = \frac{x_1 \omega e^{\gamma\varepsilon} - (\gamma\sin(\omega\varepsilon) + \omega\cos(\omega\varepsilon))x_0}{\sin(\omega\varepsilon)},$$

$$x_1 = \left(\dot{x}(0)\frac{\sin(\omega\varepsilon)}{\omega} + \left(\gamma\frac{\sin(\omega\varepsilon)}{\omega} + \cos(\omega\varepsilon)\right)x(0)\right)e^{-\varepsilon\gamma}.\qquad(6.12)$$
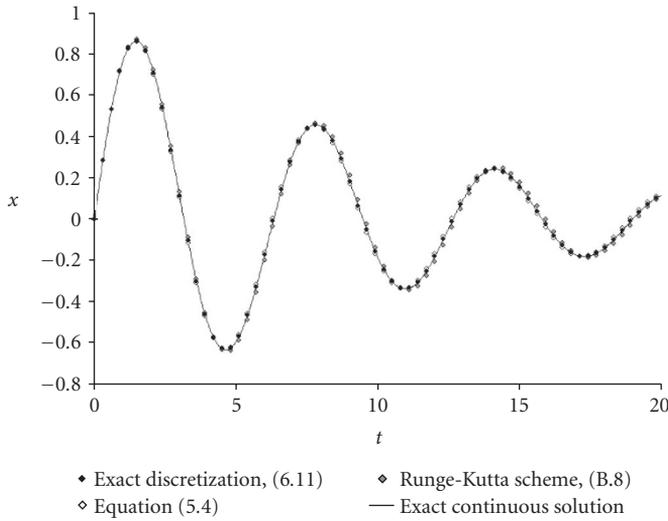
Figure 6.1. Good discretizations of the weakly damped harmonic oscillator equation ($\omega_0 = 1$, $\gamma = 0.1$) for small $t$ and $\varepsilon = 0.2$.

Figures 6.1 and 6.2 compare our exact discretization with two other good discretizations of the weakly damped harmonic oscillator. The exact discretization is really exact, that is, the discrete points belong to the graph of the exact continuous solution (for any $\varepsilon$ and any $n$). Similarly as in the undumped case, the fully symmetric simple discretization (5.4) is better than the equation resulting from the GLRK method.

The exact discretization of the harmonic oscillator equation $\ddot{x} + x = 0$ is a special case of (6.11) and is given by

$$x_{n+2} - 2(\cos\varepsilon)x_{n+1} + x_n = 0. \tag{6.13}$$

It is easy to verify that the formula (6.13) can be rewritten as

$$\frac{x_{n+2} - 2x_{n+1} + x_n}{\left(2\sin(\varepsilon/2)\right)^2} + x_{n+1} = 0, \tag{6.14}$$

which reminds the "symmetric" version of Euler's discretization scheme (see (1.2) and (2.2)), but $\varepsilon$ that appears in the discretization of the second derivative is replaced by $2\sin(\varepsilon/2)$. For small $\varepsilon$ we have $2\sin(\varepsilon/2) \approx \varepsilon$.

The solution of the initial value problem for (6.13) is given by

$$x_n = x_0\cos(n\varepsilon) + \frac{x_1 - x_0\cos\varepsilon}{\sin\varepsilon}\sin(n\varepsilon), \tag{6.15}$$

(cf. (6.8)). Thus the discrete analogue of $x(0)$ is simply $x_0$, while the initial analogue of $\dot{x}(0)$ is $(x_1 - x_0\cos\varepsilon)/\sin\varepsilon$.
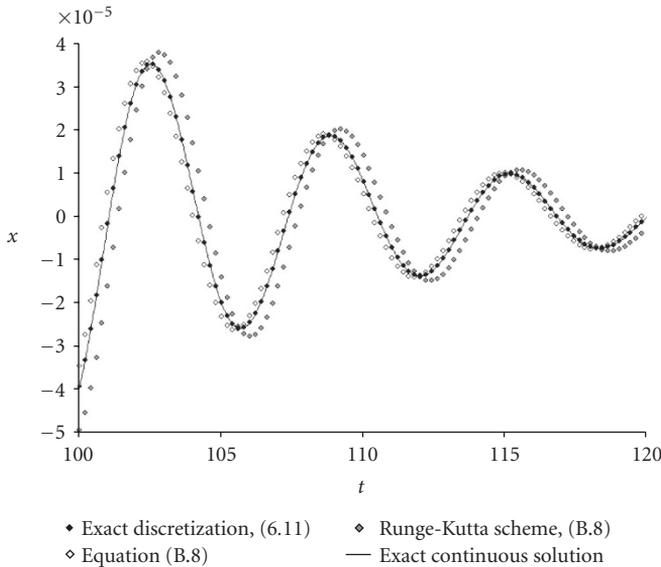
Figure 6.2. Good discretizations of the weakly damped harmonic oscillator equation ($\omega_0 = 1$, $\gamma = 0.1$) for large $t$ and $\varepsilon = 0.2$.

The comparison of the exact discretization (6.13) with three other discrete equations simulating the harmonic oscillator is done in Figures 2.3 and 4.1. We point out that the considered simulations are very good indeed (although $t$ in **Figure 2.3** is very large) but they cannot be better than the exact discretization. The discretization (4.16) is also excellent. The coefficient by $-2x_n$ in (4.16),

$$\frac{12 - 5\varepsilon^2}{12 + \varepsilon^2} \approx 1 - \frac{1}{2!}\varepsilon^2 + \frac{1}{4!}\varepsilon^4 + \cdots, \tag{6.16}$$

approximates $\cos\varepsilon$ up to the 4th order. Actually, for the choice of parameteres made in Figures 2.3 and 4.1, the discretization (4.16) practically cannot be discerned from the exact one.

## 7. Conclusions

In this paper we have shown that for linear ordinary differential equations of second order with constant coefficients, there exists a discretization which simulates properly all features of the differential equation. The solutions of this discrete equation exactly coincide with the solutions of the corresponding differential equation evaluated at a discrete lattice. Such exact discretization can be found for an arbitrary lattice spacing $\varepsilon$.

Therefore we conclude that in this case, differential and difference equations are in one-to-one correspondence: to any linear differential equation with constant coefficients there corresponds a difference equation which we call the exact discretization (such discretizations are also known as the "best" [1]). Analogical considerations can be made for linear ordinary differential equations (with constant coefficients) of any order [1, 11, 12].

We point out that to achieve our goal, we had to assume an essential dependence of the discretization on the considered equation, in contrast to the standard numerical approach to ordinary differential equations where practically no assumptions are imposed on the considered system (i.e., universal methods, applicable for any equation, are considered) [7].

In the last years one can observe the development of the numerical methods which are applicable for some clases of equations (e.g., admitting Hamiltonian formulation) but are much more powerful (especially when global or qualitative aspects are considered) [6, 13].

"Recent years have seen a shift in paradigm away from classical considerations which motivated the construction of numerical methods for ordinary differential equations. Traditionally the focus has been on the stability of difference schemes for dissipative systems on compact time intervals. Modern research is instead shifting in emphasis towards the preservation of invariants and the reproduction of correct qualitative features" [9].

In our paper we have a kind of extremal situation: the method is applicable for a very narrow class of equations but as a result we obtain the discretization which seems to be surprisingly good. Linear ordinary differential equations with constant coefficients always admit the unique exact discretization. An interesting list of other ordinary differential equations possesing the exact discretization is presented in the book [1, Chapter 3].

Similar situation occurs for integrable nonlinear partial differential equations (soliton systems). It is believed (and proved for a very large class of equations) that integrable equations admit integrable discretizations which preserve the unique features of these equations (infinite number of conservation laws, solitons, transformations generating explicit solutions, etc.) [2, 4]. It would be interesting to compare standard integrable discretizations of KdV and modKdV equations (see, e.g., [14]) with discretizations constructed in order to simulate in the best way one soliton solutions ([1]).

## Appendices

### A. Linear difference equations with constant coefficients

We recall a method of solving difference equations with constant coeficients. It consists in representing the equation in the form of a matrix equation of the first order. The general linear discrete equation of the second order,

$$x_{n+2} = 2Ax_{n+1} + Bx_n, \qquad (A.1)$$

can be rewritten in the matrix form as follows:

$$y_{n+1} = My_n, \qquad (A.2)$$

where

$$y_n = \begin{pmatrix} x_{n+1} \\ x_n \end{pmatrix}, \qquad M = \begin{pmatrix} 2A & B \\ 1 & 0 \end{pmatrix}. \qquad (A.3)$$

The general solution of (A.2) has, obviously, the following form:

$$y_n = M^n y_0, \tag{A.4}$$

and the solution of a difference equation is reduced to the purely algebraic problem of computing powers of a given matrix.

The same procedure can be applied for any linear difference equation with constant coefficients. If the difference equation is of $m$th order, then to obtain (A.2), we define

$$y_n := \left( x_{n+m}, x_{n+m-1}, \ldots, x_{n+1}, x_n \right)^T, \tag{A.5}$$

where the superscript $T$ means the transposition.

The power $M^n$ can be easily computed in the generic case in which the matrix $M$ can be diagonalized, that is, represented in the form

$$M = NDN^{-1}, \tag{A.6}$$

where $D$ is a diagonal matrix. Then, obviously, $M^n = ND^n N^{-1}$. The diagonalization is possible whenever the matrix $M$ has exactly $m$ linearly independent eigenvectors (in particular, if the characteristic equation (A.7) has $m$ pairwise different roots). Then the columns of the matrix $N$ are just eigenvectors of $M$, and the diagonal coefficients of $D$ are eigenvalues of $M$.

The characteristic equation $(\det(M - \lambda I) = 0)$ for $m = 2$ (i.e., for (A.1)) has the form

$$\Lambda^2 - 2A\lambda - B = 0. \tag{A.7}$$

Its roots will be denoted by $\Lambda_1, \Lambda_2$ (see (6.3)). If $\Lambda_1 \neq \Lambda_2$, then the diagonalization procedure yields

$$M = N \begin{pmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{pmatrix} N^{-1}, \tag{A.8}$$

where the columns of $N$ are the eigenvectors of $M$, that is,

$$N = \begin{pmatrix} \Lambda_1 & \Lambda_2 \\ 1 & 1 \end{pmatrix}. \tag{A.9}$$

Therefore

$$\begin{pmatrix} x_{n+1} \\ x_n \end{pmatrix} = N \begin{pmatrix} \Lambda_1^n & 0 \\ 0 & \Lambda_2^n \end{pmatrix} N^{-1} \begin{pmatrix} x_1 \\ x_0 \end{pmatrix}, \tag{A.10}$$

and performing the multiplication we get (6.2).

The case of multiple eigenvalues of $M$ is technically more complicated. In order to compute $M^n$ we can, for instance, transform $M$ to the Jordan canonical form (see, e.g., [8]). Here we suggest a method which is very efficient for $2 \times 2$ matrices. By the Cayley-Hamilton theorem [8], any matrix satisfies its characteristic equation. In the case of (A.1)

it means that $M^2 = 2A\lambda M + B$. In the case of the double root ($B = -A^2$) one can easily prove by induction

$$M^n = (1 - n)A^n M + nA^{n-1}. \tag{A.11}$$

Substituting it to (A.2) we get immediately (6.4).

## B. Numerical methods for ordinary differential equations

In this short note we give basic informations about some numerical methods for ordinary differential equations and we apply them to case of harmonic oscillator equation (2.4).

A system of linear ordinary differential equations (of any order) can always be rewritten as a single matrix equation of the first order:

$$\dot{y} = Sy, \tag{B.1}$$

where the unknown $y$ is a vector and $S$ is a given matrix (in general $t$-dependent). Numerical methods are almost always (see [7]) constructed for a large class of ordinary differential equations (including nonlinear ones):

$$\dot{y} = f(t, y). \tag{B.2}$$

We denote by $y_n$ a numerical approximant to the exact solution $y(t_n)$.

*Euler's method.*

$$y_{k+1} = y_k + \varepsilon f(t_k, y_k). \tag{B.3}$$

In this case the discretization of $\ddot{x} + x = 0$ is given by (2.1).

*Modified Euler's methods.*

$$y_{k+1} = y_k + \varepsilon f\left(t_k + \frac{1}{2}\varepsilon, y_k + \frac{1}{2}\varepsilon f(t_k, y_k)\right),$$

$$y_{k+1} = y_k + \frac{1}{2}\varepsilon(f(t_k, y_k) + f(t_k + \varepsilon, y_k + \varepsilon f(t_k, y_k))). \tag{B.4}$$

Both methods lead to the following discretization of $\ddot{x} + x = 0$:

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\varepsilon^2} + x_n + \frac{1}{4}\varepsilon^2 x_{n-1} = 0. \tag{B.5}$$

The roots of the characteristic equation are imaginary and

$$|\Lambda_1| = |\Lambda_2| = \sqrt{1 + \frac{\varepsilon^4}{4}}. \tag{B.6}$$

*1-stage Gauss-Legendre-Runge-Kutta method.*

$$y_{k+1} = y_k + \varepsilon f\left(t_k + \frac{1}{2}\varepsilon, \frac{y_k + y_{k+1}}{2}\right). \tag{B.7}$$

The application of this numerical integration scheme yields the following discretization of the damped harmonic oscillator equation:

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\varepsilon^2} + 2\gamma \frac{x_{n+1} - x_{n-1}}{2\varepsilon} + \omega_0^2 \frac{x_{n+1} + 2x_n + x_{n-1}}{4} = 0. \tag{B.8}$$

In the case $\gamma = 0$, $\omega_0 = 1$ (i.e., $\ddot{x} + x = 0$), we have

$$\Lambda_1 = \frac{2 + i\varepsilon}{2 - i\varepsilon}, \qquad \Lambda_2 = \frac{2 - i\varepsilon}{2 + i\varepsilon}. \tag{B.9}$$

*Adams-Bashforth extrapolation formula.*

$$y_{n+1} = y_n + \varepsilon \sum_{j=0}^{k} b_{kj} f\left(t_{n-j}, y_{n-j}\right), \tag{B.10}$$

where $b_{kj}$ are specially chosen real numbers. In particular, $b_{10} = 3/2$, $b_{11} = -1/2$, $b_{20} = 23/12$, $b_{21} = -4/3$, $b_{22} = 5/12$.

In the case $k = 1$, we obtain (for $\ddot{x} + x = 0$)

$$\frac{x_{n+1} - 2x_n + x_{n-1}}{\varepsilon^2} + \frac{9x_{n-1} - 6x_{n-2} + x_{n-3}}{4} = 0 \tag{B.11}$$

and the characteristic equation reads

$$\Lambda^4 - 2\Lambda^3 + \left(1 + \frac{9}{4}\varepsilon^2\right)\Lambda^2 - \frac{3}{2}\varepsilon^2\Lambda + \frac{1}{4}\varepsilon^2 = 0. \tag{B.12}$$

This is an equation of the 4th order (with no real roots for $\varepsilon \neq 0$).

## Acknowledgment

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